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Pin-Pointing Solution of Ill-Conditioned Square Systems of Linear Equations

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Abstract—A new method is proposed for an accurate solution of nearly singular systems of linear equations. The method uses the truncated singular value decomposition of the initial coefficient matrix at the first stage and the Gaussian elimination procedure for a well-conditioned reduced system of linear equations at the last stage. In contrast to various regularization techniques, the method does not require any additional physical information on the problem. © 2000 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

There are various direct and iterative approaches to solve square systems of linear algebraic equations

$$A\mathbf{x} = \mathbf{b}, \tag{1}$$

where A is an $m \times m$ coefficients' matrix and $\mathbf{x}$ and $\mathbf{b}$ are vectors of unknowns and right-hand sides, correspondingly. Unfortunately, existing methods may lead to inaccurate solution of (1) where matrix A is ill conditioned. The latter happens rather frequently in physics, engineering, and other branches of science. Solving (1) with standard software, the following warning: "results for solution of ill-conditioned matrix may contain significant numerical error", often appears. The obvious method of overcoming this problem is to scale matrix A appropriately. However, " ... the

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scaling of equations and unknowns must proceed on a problem-by-problem basis, general scaling strategies are unreliable" [1].

Another approach to solution of (1) is to consider the problem as a particular case of the least squares (LS) problem: $\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|_2$. This reformulation allows one to adopt various numerical techniques typical of LS problems [2]. These techniques are mostly based on various rank revealing decompositions of matrix A. Among them, the singular value decomposition (SVD) is the most general and reliable. The SVD of the coefficients' matrix takes the form

$$A = V\Sigma U^\top = \sum_{i=1}^{m} \sigma_i \mathbf{v}_i \mathbf{u}_i^\top, \tag{2}$$

where Σ is an $m \times m$ diagonal matrix of singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m > 0$ and V and U are square matrices formed of left ($\mathbf{u}_i$) and right ($\mathbf{v}_i$) singular vectors. By using (2), the solution of (1) takes the form

$$\mathbf{x} = \sum_{i=1}^{m} \sigma_i^{-1} \mathbf{u}_i \left(\mathbf{v}_i^\top \mathbf{b}\right). \tag{3}$$

The weak point of the SVD solution is the inaccurate computation of small singular values. "What to do with small but significant singular values is a difficult and unsolved problem" [3]. However, the small singular values are inherent in the SVD of badly conditioned matrices and, consequently, solution (3) may not be accurate.

Intuition suggests that existing algorithms collapse in solving ill-conditioned problems at some stage where "nearness" of the initial coefficient matrix columns (rows) becomes crucial. The algorithm presented in this work is an attempt to bypass computations in the "dangerous domains" and to provide an accurate solution to the problem.

2. THE ALGORITHM

Let the following "dangerous" small singular values be neglected in the SVD solution:

$$\epsilon > \sigma_{n+1} \geq \sigma_{n+2} \geq \cdots \geq \sigma_m. \tag{4}$$

Then (3) takes the form

$$\mathbf{x}_1 = \sum_{i=1}^{n} \sigma_i^{-1} \mathbf{u}_i \left(\mathbf{v}_i^\top \mathbf{b}\right). \tag{5}$$

Parameter ϵ defines version of the truncated SVD (TSVD). The TSVD solution (5) is widely used as a regularized LS problem solution [4]. For the purpose of this paper, however, solution (5) is not accurate enough. It may be pin-pointed in the following way.

Let the matrices of the left and right singular vectors of the TSVD be designated as $V_1 = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ and $U_1 = [\mathbf{u}_1, \dots, \mathbf{u}_n]$, then their orthogonal complements are $\tilde{V}_2 = [\tilde{\mathbf{v}}_{n+1}, \dots, \tilde{\mathbf{v}}_m] \equiv V_1^{(\perp)}$ and $\tilde{U}_2 = [\tilde{\mathbf{u}}_{n+1}, \dots \tilde{\mathbf{u}}_m] \equiv U_1^{(\perp)}$, correspondingly. Columns of matrices $\tilde{V}_2$ and $\tilde{U}_2$ span nullspaces of matrices $V_1^\top$ and $U_1^\top$. Instead of using singular vectors of the full SVD corresponding to neglected singular values, it is preferable to compute orthonormal sets $\tilde{\mathbf{v}}_{n+1}, \dots, \tilde{\mathbf{v}}_m$ and $\tilde{\mathbf{u}}_{n+1}, \dots, \tilde{\mathbf{u}}_m$ on the base of "good" matrices $V_1^\top$ and $U_1^\top$. It may be carried out in various ways as shown in the next section.

Splitting the unknowns in (2) as follows:

$$\mathbf{x} = U_1 \mathbf{z}_1 + \tilde{U}_2 \mathbf{z}_2 \tag{6}$$

and multiplying (1) by $[V_1, \tilde{V}_2]^\top$ from the left, (1) takes the form

$$\tilde{A}\mathbf{z} = \begin{bmatrix} \operatorname{diag}(\sigma_1, \dots, \sigma_n) & 0 \\ 0 & C \end{bmatrix} \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}, \tag{7}$$

in which

$$\begin{aligned} \tilde{A} &= \left[V_1, \tilde{V}_2\right]^{\mathsf{T}} A \left[U_1, \tilde{U}_2\right], \\ C &= \tilde{V}_2^{\mathsf{T}} A \tilde{U}_2, \\ \mathbf{b}_1 &= V_1^{\mathsf{T}} \mathbf{b}, \qquad \mathbf{b}_2 = \tilde{V}_2^{\mathsf{T}} \mathbf{b}. \end{aligned} \tag{8}$$

The new system of linear equations (7) is solved independently for $\mathbf{z}_1$ and $\mathbf{z}_2$. Vector $\mathbf{z}_1$ corresponds to the TSVD solution discussed above,

$$U_1 \mathbf{z}_1 = \mathbf{x}_1 \tag{9}$$

and vector $\mathbf{z}_2$ is computed from the following equation:

$$C \mathbf{z}_2 = \mathbf{b}_2. \tag{10}$$

This may be done by using the Gaussian Elimination (GE) procedure. It is important to note that an $m - n \times m - n$ matrix C is well conditioned in contrast to matrix A. Indeed, the singular values of matrix C are the neglected small singular values of matrix A:

$$\begin{aligned} C = \tilde{V}_2^{\mathsf{T}} A \tilde{U}_2 &= \tilde{V}_2^{\mathsf{T}} \left[V_1, V_2\right] \operatorname{diag}(\sigma_1, \ldots, \sigma_m) \left[U_1, U_2\right]^{\mathsf{T}} \tilde{U}_2 \\ &= \left(\tilde{V}_2^{\mathsf{T}} V_2\right) \operatorname{diag}(\sigma_{n+1}, \ldots, \sigma_m) \left(U_2^{\mathsf{T}} \tilde{U}_2\right), \end{aligned} \tag{11}$$

in which $V_2 = [\mathbf{v}_{n+1}, \ldots, \mathbf{v}_m]$ and $U_2 = [\mathbf{u}_{n+1}, \ldots, \mathbf{u}_m]$. Since matrices in the parentheses on the right-hand side of (11) are orthogonal, then the right-hand side of (11) is the SVD of matrix C. Consequently, designating the 2-norm condition number as κ_2, we have:

$$\kappa_2(A) = \|A\|_2 \left\|A^{-1}\right\|_2 = \sigma_1 \sigma_m^{-1}, \tag{12}$$

$$\kappa_2(C) = \|C\|_2 \left\|C^{-1}\right\|_2 = \sigma_{n+1} \sigma_m^{-1}, \tag{13}$$

and

$$\frac{\kappa_2(C)}{\kappa_2(A)} = \frac{\sigma_{n+1}}{\sigma_1} < \varepsilon \sigma_1^{-1} \ll 1. \tag{14}$$

3. IMPLEMENTATION

The proposed scheme for solving ill-conditioned square systems of linear equations consists of three steps.

1. Compute the TSVD: $\sigma_1, \ldots, \sigma_n, U_1, V_1$.
2. Compute $\tilde{U}_2 = \operatorname{null}(U_1^{\mathsf{T}})$ and $\tilde{V}_2 = \operatorname{null}(V_1^{\mathsf{T}})$ and C.
3. Compute solution of (10) and to obtain the final answer by using (6).

Every step may be carried out by using such standard software packages as Mathematica [5] or Matlab [6], for example. Both programs are based on the Linpack package [3]. There is a difference between Mathematica and Matlab in the location of the nullspace for the second step of the proposed scheme. Matlab's "null" procedure uses Linpack's QR decomposition with Householder reflectors [3, Chapter 9], while Mathematica's numerical "NullSpace" procedure uses Linpack's SVD [3, Chapter 11].

4. TEST

Consider 14×14 Hilbert matrix: $H_{ij} = 1/(i + j - 1)$, $i, j = 1, \ldots, 14$. Let this matrix be designated as H_{14}^{16} in decimal notation with precision of 16 digits. H_{14}^{16} is a singular matrix since it is possible to calculate its nontrivial nullspace. This means that H_{14}^{16} is unacceptable for testing.

Table 1. $\mathbf{b}_1 = \{1,0,0,0,0,0,0,0,0,0,0,0,0,0\}$.

Exact Solution	Proposed Scheme	Gaussian Elimination	SVD
196	196	87.0041	127.222
−19110	−19110	−2994.77	−8012.95
611520	611520	17557.3	162904
−9529520	−9.52952 E6	23242.	−1.56292 E6
85765680	8.57657 E7	2.24818 E6	8.21321 E6
−488864376	−4.88864 E8	−4.49157 E7	−2.49778 E7
1862340480	1.86234 E9	3.35529 E8	4.28056 E7
−4888643760	−4.88864 E9	−1.37766 E9	−3.25868 E7
8962513560	8.96251 E9	3.50216 E9	−1.05463 E7
−11452100660	−1.14521 E10	−5.76064 E9	3.30319 E7
9994560576	9.99456 E9	6.1563 E9	−1.36719 E6
−5678727600	−5.67873 E9	−4.13329 E9	−3.31957 E7
1892909200	1.89291 E9	1.58543 E9	2.68163 E7
−280816200	−2.80816 E8	−2.65193 E8	−6.78517 E6

Table 2. $\mathbf{b}_{14} = \{0,0,0,0,0,0,0,0,0,0,0,0,0,1\}$.

Exact Solution	Proposed Scheme	Gaussian Elimination	SVD
−280816200	−2.80816 E8	−2.42953 E8	−6.78517 E6
51108548400	5.11085 E10	3.1688 E10	7.92154 E8
−2299884678000	−2.29988 E12	−9.8841 E11	−2.25417 E10
44975522592000	4.49755 E13	1.25109 E13	2.70756 E11
−477864927540000	−4.77865 E14	−7.3959 E13	−1.68048 E12
3096564730459200	3.09656 E15	1.62634 E14	5.83812 E12
−13074384417494400	−1.30744 E16	4.3764 E14	−1.12518 E13
37355384049984000	3.73554 E16	−3.98702 E15	9.85468 E12
−73543412348406000	−7.35434 E16	1.24898 E16	2.03931 E12
99873769855860000	9.98738 E16	−2.24419 E16	−9.98297 E12
−91883868267391200	−9.18839 E16	2.50689 E16	1.28701 E12
54674698473158400	5.46747 E16	−1.72425 E16	1.01715 E13
−18984270303180000	−1.89843 E16	6.70542 E15	−8.88513 E12
2920656969720000	2.92066 E15	−1.13054 E15	2.36075 E12

However, the precision of 17 digits (available by Mathematica) leads to the following nonsingular and very ill-conditioned matrix H_{14}^{17} which is acceptable for testing: $\kappa_2(H_{14}^{17}) \sim 10^{19}$.

The testing strategy was to solve equation $H_{14}^{17}\mathbf{x}_i = \mathbf{b}_i$ for various $\mathbf{b}_i$. Particularly, solutions were obtained for 14 r.h.s. vectors: $\mathbf{b}_i = \{0,\dots,0,1(i),0,\dots,0\}$, $i = 1,\dots,14$. In other words, the inverse $(H_{14}^{17})^{-1}$ was computed.

Tables 1 and 2 present solutions for $\mathbf{b}_1$ and $\mathbf{b}_{14}$ typical of the rest of right-hand sides. The first column of the tables shows exact solution for exact matrix H_{14} obtained in integers. The second column presents solution for H_{14}^{17} in accordance with the proposed scheme ($\varepsilon = 10^{-8}$). The third and the fourth columns present GE (with partial pivoting) and SVD solutions for H_{14}^{17}, correspondingly. All computations were carried out in Mathematica 2.2.

Taking into account that the considered Hilbert matrix belongs to the class of Cauchy matrices for which fast and accurate solution procedures have been developed [7], it is reasonable to use for testing some matrix which does not enjoy Cauchy structure. The following 14×14 matrix (given by rows) was used:

$$
\begin{aligned}
F = \{&\{1/9, 1/12, 1/15, 1/3, 1/7, 1/10, 1/13, 1/16, 1/5, 1/8, 1/11, 1/14, 1/17, 1/6\},\\
&\{1/13, 1/16, 1/19, 1/8, 1/11, 1/14, 1/17, 1/20, 1/9, 1/12, 1/15, 1/18, 1/21, 1/10\},\\
&\{1/17, 1/20, 1/23, 1/12, 1/15, 1/18, 1/21, 1/24, 1/13, 1/16, 1/19, 1/22, 1/25, 1/14\},\\
&\{1/7, 1/10, 1/13, 1, 1/5, 1/8, 1/11, 1/14, 1/3, 1/6, 1/9, 1/12, 1/15, 1/4\},\\
&\{1/11, 1/14, 1/17, 1/6, 1/9, 1/12, 1/15, 1/18, 1/7, 1/10, 1/13, 1/16, 1/19, 1/8\},\\
&\{1/15, 1/18, 1/21, 1/10, 1/13, 1/16, 1/19, 1/22, 1/11, 1/14, 1/17, 1/20, 1/23, 1/12\},\\
&\{1/19, 1/22, 1/25, 1/14, 1/17, 1/20, 1/23, 1/26, 1/15, 1/18, 1/21, 1/24, 1/27, 1/16\},\\
&\{1/22, 1/25, 1/28, 1/17, 1/20, 1/23, 1/26, 1/29, 1/18, 1/21, 1/24, 1/27, 1/30, 1/19\},\\
&\{1/10, 1/13, 1/16, 1/5, 1/8, 1/11, 1/14, 1/17, 1/6, 1/9, 1/12, 1/15, 1/18, 1/7\},\\
&\{1/14, 1/17, 1/20, 1/9, 1/12, 1/15, 1/18, 1/21, 1/10, 1/13, 1/16, 1/19, 1/22, 1/11\},\\
&\{1/18, 1/21, 1/24, 1/13, 1/16, 1/19, 1/22, 1/25, 1/14, 1/17, 1/20, 1/23, 1/26, 1/15\},\\
&\{1/8, 1/11, 1/14, 1/2, 1/6, 1/9, 1/12, 1/15, 1/4, 1/7, 1/10, 1/13, 1/16, 1/5\},\\
&\{1/21, 1/24, 1/27, 1/16, 1/19, 1/22, 1/25, 1/28, 1/17, 1/20, 1/23, 1/26, 1/29, 1/18\},\\
&\{1/16, 1/19, 1/22, 1/11, 1/14, 1/17, 1/20, 1/23, 1/12, 1/15, 1/18, 1/21, 1/24, 1/13\}\}
\end{aligned}
$$

The appropriate test results for this matrix are given in Tables 3 and 4. Though the exact solution in the first column of Tables 3 and 4 are given in decimal notation, they were obtained actually in integers and complex final fractions were presented in decimal notation.

Table 3. $\mathbf{b}_1 = \{1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$.

Exact Solution	Proposed Scheme	Gaussian Elimination	SVD
3.49297 E11	3.49297 E11	3.19750 E10	8.92367 E9
−5.83512 E12	−5.83512 E12	5.25099 E10	4.89854 E9
3.36406 E12	3.36406 E12	−2.50852 E11	1.20914 E10
13.2278	13.2278	13.6683	13.8984
6.86703 E9	6.86703 E9	1.32043 E9	5.51605 E8
−1.29412 E12	−1.29412 E12	−6.82223 E10	−1.47831 E10
7.21593 E12	7.21593 E12	−2.43877 E11	−1.13560 E10
−1.08984 E12	−1.08984 E12	9.96847 E10	−9.180609 E9
9.55282 E6	9.55282 E6	3.24324 E6	1.87020 E6
−6.23388 E10	−6.23388 E10	−8.56798 E9	−2.96481 E9
3.29000 E12	3.29000 E12	6.43596 E10	1.02860 E10
−6.10172 E12	−6.10172 E12	3.38536 E11	−6.58395 E8
1.57392 E11	1.57392 E11	−1.67639 E10	2.24209 E9
−4.08904 E8	−4.08904 E8	−1.05724 E8	−5.22859 E7

5. DISCUSSION

Numerical tests show excellent accuracy of the proposed scheme while traditional approaches collapse. Since the proposed scheme consists of several steps which include the standard numerical procedures as SVD, QR decomposition, GE, then the general *backward stability* analysis leans for support on the corresponding analyses of every procedure used. They may be found in [1,2,8]. The accuracy, or small *forward error*, of the proposed scheme is due to the use of TSVD instead of SVD at the first step and a well-conditioned matrix C at the last step.

The proposed scheme is rich in computations. This is a payment for its accuracy. On the other hand, this scheme is easily implemented by the public domain software. The latter may be an attractive and crucial merit for solving ill-conditioned systems practically.

Table 4. $\mathbf{b}_{14} = \{0,0,0,0,0,0,0,0,0,0,0,0,0,1\}$.

Exact Solution	Proposed Scheme	Gaussian Elimination	SVD
−3.02563 E17	−3.02563 E17	6.23789 E14	1.62979 E13
5.84529 E18	5.84529 E18	−3.57370 E16	8.78658 E12
−3.70222 E18	−3.70222 E18	3.40728 E16	2.48387 E13
320627	320627	7668.04	−1385.02
−5.10942 E15	−5.10942 E15	−7.22054 E12	8.88858 E11
1.18626 E18	1.18626 E18	−4.20540 E15	−2.84283 E13
−7.48974 E18	−7.48974 E18	5.41699 E16	−2.32615 E13
1.22906 E18	1.22906 E18	−1.23835 E16	−1.94728 E13
−5.56654 E12	−5.56654 E12	−3.21084 E10	2.46532 E9
5.04399 E16	5.04399 E16	−2.10675 E13	−5.11597 E12
−3.16348 E18	−3.16348 E18	1.54686 E16	2.11455 E13
6.53322 E18	6.53322 E18	−5.39563 E16	−4.58608 E11
−1.81427 E17	−1.81427 E17	1.97453 E15	4.85434 E12
2.73668 E14	2.73668 E14	9.47571 E11	−7.72604 E10

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